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LEAST SQUARES SURFACE APPROXIMATION
TO SCATTERED DATA USING
MULTIQUADRIC FUNCTIONS

by

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9 ABSTRACT (Continue on reverse if necessary and identify by block number) This report documents an investigation into some methods for fitting surfaces to scattered data. The form of the fitting function is a multiquadric function with the criteria for the fit being the least mean squared residual for the data points. The principal problem is the selection of knot points (or base points for the multiquadric basis functions), although the selection of the multiquadric parameter also plays a nontrivial role in the process. We first describe a greedy algorithm for knot selection, and this procedure is used as an initial step in what follows. The minimization (including knot locations and multiquadric parameter is explored, with some unexpected results in terms of "near repeated" knots. This phenomenon is explored, and leads us to consider variable parameter values for the basis functions. Examples and results are given throughout.					
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1.0 Introduction

This report concerns the use of multiquadric functions to approximate scattered data. Here we deal with functions of two independent variables, but the methods are easily extendible to arbitrary dimensions, and we expect that many of the conclusions will carry over.

The impetus behind our investigation is that of obtaining surface approximations that are efficient in subsequent applications. That is, we consider it to be acceptable to expend considerable computational resources to obtain the approximation in a preprocessing step. Once obtained, the approximation should be able to be evaluated fairly efficiently such as when it is to be used numerous times in an application program.

The scattered data approximation problem is easily described and occurs frequently in many branches of science. The problem occurs in any discipline where measurements are taken at irregularly spaced values of two or more independent variables, and is especially prevalent in environmental sciences. We will suppose that triples of data, (x_j, y_j, z_j) , $j=1, \dots, N$ are given, assumed to be measurements (perhaps with error) of an underlying function $z=f(x,y)$. The function f is to be approximated by a function $F(x,y)$ from the given data. A recent survey of such methods is given in [FN91].

Multiquadric functions were introduced for interpolation of scattered data by Hardy [HA71]; also see [HA92] for a historical survey and many references. The method is one of a class of methods known now as "radial basis function methods" that includes other attractive schemes such as thin plate splines [HD71, DU76, and others]. The basic idea of such methods is quite simple, and we describe it in some generality; for purposes of being definite it is pertinent to note that for the multiquadric method the radial function is $h(d) = \sqrt{d^2 + r^2}$. In general, suppose a function of one variable, $h(d)$, where d denotes distance, is given.

For interpolation (that is, exact matching of the given data), a basis function, $B_j(x,y) = h(d_j)$ is associated with each

data point. Here $d_j = \sqrt{(x-x_j)^2+(y-y_j)^2}$, distance from (x,y) to (x_j,y_j) . Thus each basis function is a translate of the radial function, h . The approximation is a linear combination of the basis functions, along with some polynomial terms that may be necessary in some cases, or may be used to assure that the approximation method has polynomial precision. Thus,

$$(1) \quad F(x,y) = \sum_{j=1}^N a_j B_j(x,y) + \sum_{j=1}^M b_j q_j(x,y)$$

where $\{q_j\}$ is a set of M polynomials forming a basis for polynomials of degree $< m$. The coefficients a_j and b_j are determined by the linear system of equations prescribing interpolation of the data, and exactness for polynomials of degree $< m$:

$$(2) \quad \begin{aligned} & \sum_{j=1}^N a_j B_j(x_i, y_i) + \sum_{j=1}^M b_j q_j(x_i, y_i) = z_i, \quad i=1, \dots, N \\ & \sum_{j=1}^N a_j q_i(x_j, y_j) = 0, \quad i=1, \dots, M. \end{aligned}$$

For multiquadric basis functions, this system of equations is known to have a unique solution for distinct (x_j, y_j) data (see, for example, [MI86]); while m may be taken as zero (no polynomial terms), the theory indicates that a constant term should be included, and we have done so in all our work. If higher degree polynomial precision is desired, inclusion of those terms imposes no particular burden.

While interpolation theory is important and indicates something about the suitability of the class of functions for approximation purposes, our emphasis here is on least squares approximation. This implies using fewer basis functions than there are data points. In analogy with univariate cubic splines, it is convenient to refer to the points at which the radial basis functions are centered as "knots", as was done in [MF92], and we do so here. If a set of knot points, (u_k, v_k) , $k=1, \dots, K$, with $K < N$ have been specified, then the problem of fitting a

multiquadric function by least squares is similar to that of solving the system of equations corresponding to those above in the least squares sense. We give the details. Now, let $B_k(x,y)$ denote the radial basis function associated with the point (u_k, v_k) , $B_k(x,y) = \sqrt{((x-u_k)^2 + (y-v_k)^2)}$. The system of equations, specialized for our case, is now of the form

$$\begin{aligned} & \sum_{k=1}^K a_k B_k(x_i, y_i) + \sum_{j=1}^M b_j q_j(x_i, y_i) = z_i, \quad i=1, \dots, N \\ (3) \quad & \sum_{k=1}^K a_k = 0. \end{aligned}$$

There is a question of how to treat the last equation, which guarantees polynomial precision. In [FC92] the corresponding constraint equations were imposed exactly, rather than approximately because of physical considerations. While there is not the corresponding physical situation here, we have also imposed the last equation as a constraint. This constraint can be used to reduce the size of the system by solving for a_K in terms of the other a_k and substituting into the first set of equations.

If the knot points are a subset of the data points, then the same theory that assures a unique solution of the system for interpolation also guarantees a unique solution of the least squares problem. When the knot locations may differ from the data points, the problem of whether the coefficient matrix is of full rank or not is unknown to us, although we feel certain that the matrix is of full rank when the knot points are distinct, and have encountered no situations that indicate otherwise.

In our implementation of the algorithms described in subsequent sections we have used a QRP' decomposition of the coefficient matrix to solve the least squares problem. This provides a stable and efficient means for solution of the problem with an indication if a matrix of less than full rank is encountered.

In order to test the algorithms we have used a number of

data sets. Several of these are based on previously published and widely available (x,y) data sets and parent functions. We have also used a few less readily available data sets that we are willing to share with anyone interested in obtaining them. Table 1 gives a summary of most of the data set.

n.m	This refers to point set n and function m from [FR82], for n=1, 2, and 3, and m=1, ..., 6. n=1 is 25 points, n=2 is 33 points, n=3 is 100 points. n=4 refers to the 200 point data set used in [MF92]. m=1 is the humps and dip function, m=2 is the cliff, m=3 is the saddle, m=4 is the gentle hill, m=5 is the steep hill, and m=6 is the sphere. In addition, m=7 refers to the curved valley function from [NI78].
GT	This refers to the thinned glacier data consisting of 678 points, with certain contour lines removed, from [MF92].
GL	This refers to the thinned glacier data consisting of 873 points.
HF	This is the data set from [MF92] generated to be approximately proportional to curvature, consisting of 500 points.

Table 1: Data sets used extensively in tests

Section 2 deals with a "greedy" algorithm for determining the location of a reasonable set of knots for approximation of given data by a least squares multiquadric function. Some experiences with the method are given. In Section 3 we expand the algorithm to include the knot locations and the parameter value of the method as part of the optimization process. Some results and observations about the process are made, with the

optimized value of the parameter r being of interest. The occurrence of near multiple knots is a particularly interesting phenomenon. In section 4 we further extend the algorithm to include variable parameter values at the knots. The optimized r_k values and the near multiple knots are again of special interest. Finally, in Section 5 we discuss some ideas for further exploration of least squares multiquadric approximations.

2.0 An Adaptive Method for Knot Selection

This section describes a greedy method for the selection of knot locations for fitting surfaces to scattered data using a least squares multiquadric function. As noted in the introduction, the use of fixed knots and parameter value with the multiquadric function results in a linear system to be solved in the least squares sense. These are solved using the QRP' decomposition. The algorithm was implemented in Matlab¹, giving access to powerful matrix-vector notation that simplifies many aspects of the implementation. In addition, Matlab allows easy interactive intervention in the process, with tabular and graphical information being made available as the computations proceeds. While an efficient implementation would also provide for updating the QRP' decomposition as more knots are added, we have not done this in the experimental program since our computational resources were sufficient to make it unnecessary.

2.1 The Algorithm

The algorithm proceeds as follows, with the necessary input being obtained by interrogation of the user. The description given starts after all input has been obtained.

- a) The initial step is to obtain the least squares fit by a constant function, the average of the data values. The two data points having maximum positive and maximum negative error are taken to be the first two knots, (u_1, v_1) and (u_2, v_2) . The knot counter K is set to 2.

¹ MathWorks, 24 Prime Park Way, Natick. MA 01760

- b) The least squares multiquadric fit with K knots is obtained. The residuals are computed along with their rms value, the approximation is evaluated on a grid of points, a smoothness measure approximately equal to the value of the thin plate functional over the region is computed, and if the underlying function is known the rms error on the grid is computed. These values are then output and a perspective plot of the approximating surface is given.
- c) The maximum absolute value of the residuals is found and the location of this residual, subject to the minimum knot separation value, is taken to be the next knot location (u_K, v_K) . At this point the algorithm proceeds to step b unless the maximum number of knot locations to be computed has been reached.

At the termination of the program, the user can restart the process with any of the parameters changed, with any number of knot point locations, up to the total number that have been computed. Hard copy plots of the surfaces and tabular output can be obtained.

2.2 Some Results

One of the interesting aspects of the multiquadric method concerns appropriate choice of the parameter, r . Initial advice was to specify the value in terms of approximate data point separation [HA71,FR82], although even in [FR82] it was clear that the best value was dependent on the ordinate data as well. More recent work [TA85, CF91] has shown this to be the case and an algorithm for a "good" value was given in [CF91].

While no algorithm was implemented to obtain the best r value for fixed knots found by the adaptive method above, the flexibility of the implementation allowed for some interactive experimentation along these lines. In most cases investigated, it was found that the value of r used in the process of selecting the knot locations also was very close to the "best" value (that is the one that minimized the rms error of the residuals) for

that particular set of knot locations. Exceptions were when the number of knots was quite small ($5 \approx 8$), in which case the multiquadric method shows a striking affinity for best fits with r very close to zero. Of course, most surfaces with any complexity cannot be fit well with so few knots. Apparently the adaptive knot selection process is quit dependent on the r value used, at least enough to rule out significant improvement by changing r once the knots have been selected.

While a reasonable a priori choice of the parameter r in this context can be made, the value of the best r is still an open question, and is not likely to be resolved anytime soon. As is pointed out by [CF91], the parameter can be used somewhat like a tension parameter (small values correspond to "tighter" surfaces), and consequently surfaces that involve steep gradients will be approximated with less overshoot by selecting a small value of r . The tension effects are limited compared with the results that can be obtained using thin plate splines with tension (see [FR85]). Other factors enter into the selection of the r value, however, since small values also lead to rapid changes in the gradient which may be undesirable.

One of the parameters in the knot selection process is the minimum separation between knots. It has been found that there is often an improvement by requiring some moderate separation between knots, for example imposing a minimum separation of .1 or .2 for 20 knots on the $[0,1]^2$ for point set 3. This tends to distribute knots more uniformly throughout the region, even when there are clumps of data. For comparison purposes, the rms errors (rmse) at the data points and over a 20×20 grid were computed and are given in Table 2 for several data sets. All 3.m examples were with $r=0.3$ and 20 knot points, while the HF data set used $r=0.2$ and 50 knot points.

data set	minsep	rmse(data)	rmse(grid)
3.1	0.0	0.0215	0.0231
	0.1	0.0262	0.0281
	0.2	0.0210	0.0241
3.2	0.0	0.0122	0.0132
	0.1	0.0162	0.0168
	0.2	0.0116	0.0133
3.3	0.0	0.0020	0.0023
	0.1	0.0014	0.0018
	0.2	0.0016	0.0019
3.6	0.0	0.0033	0.0038
	0.1	0.0026	0.0031
	0.2	0.0053	0.0051
HF	0.0	0.0031	0.0040
	0.05	0.0030	0.0037
	0.1	0.0032	0.0045

Table 2: rms errors for various separation distances

In the case given in [MF92] where the data was specifically generated to reflect the curvature of the underlying surface, the knots computed by this algorithm tend to be gathered in regions where the density of data points is greatest. Figure 1 gives the results in one case. It shows the data points and the subset selected as knot points by the greedy algorithm, along with the contours of the parent surface, in part a. Here the minimum separation distance of 0.05 was imposed, resulting in a more regular distribution than when a zero separation distance is imposed. In part b the surface from which the data was sampled

is shown. This function is used in later examples (function 1 from the table); the viewpoint is from the right center field. In part c the surface shown is that constructed by least squares fit using the knot points in part a. Part d shows the contours of the approximating surface. Part a can be directly compared with Figure 3 in [MF92], and it is seen that the distribution is different, and in particular does not have the nice spacing of that in [MF91]. Qualitatively the knot locations given here do reflect the density of the data, however.

The greedy algorithm given here appears to be potentially useful for many problems where data subject to error is available and the surface must be approximated using an approximation that is computationally as efficient as possible. A problem which we have considered, but which needs additional attention, is that of when enough knots have been generated so that the behavior of the underlying surface is captured without undue influence by the errors in the data. For now, this is mostly an unexplored idea, and we have more to say about it in Section 5.

3.0 Variable Knot Locations and Multiquadric Parameter

While the adaptive method discussed in the previous section seemed to perform reasonably well, it was felt prudent to check the performance of the scheme against one which considered the knot locations, along with the parameter value, r , to be variables over which the minimization of rms errors at the data points was achieved. The function to be minimized in this case is the same as before, but here we will state it explicitly rather than in the implied form where the least squares solution was that of the overdetermined system (3). The minimization problem is

$$(4) \quad \min \sum_{i=1}^N [z_i - \sum_{k=1}^K a_k B_k(x_i, y_i) - c]^2$$

where the minimization is taken over all (u_k, v_k) , r , the a_k , and c (with the last equation of (3) imposed as a constraint). As a practical matter, for each given knot configuration and r value,

the least squares solution of (3) computed as a step toward (4). This results in the solution of a simpler, but equivalent problem since $2K$ parameters are eliminated from (4) by imposing the condition that the values of the a_j and c be always taken as obtained from the least squares solution of (3). Hence, our final process is more properly written as

$$(5) \quad \min \min_{i=1}^N \sum_{k=1}^K [z_i - \sum_{k=1}^K a_k B_k(x_i, y_i) - c]^2$$

where the inner minimization is over the a_j and c (least squares solution of (3)), and the outer minimization is over the knot locations and the value of the parameter r . The global minimum of each of the two problems are clearly the same. Eq. (5) is the more restrictive, but any minimum of (4) is a local minimum of (5), else a better solution is attainable for (4). This does not imply that the iterative methods employed to solve (5) would work equally well, nor find the same local minima, when applied to (4).

When knot locations are allowed to differ from data locations, the guarantee of full rank of the coefficient matrix conferred on the system by interpolation theory no longer holds. As we noted in the Introduction, this has not posed any problems in our computations.

3.1 Optimization Algorithms and Initial Guesses

We have used two different nonlinear optimization schemes, both implemented and available as part of Matlab. One is the procedure FMINS that is based on a simplex procedure [W085]. The other is LEASTSQ that is based on the Levinberg-Marquardt procedure. Both of the routines appear to reliably find good local minima that are qualitatively similar, although LEASTSQ often finds a somewhat smaller rms residual and we have used it for most of the results given here.

The initial guess has a strong influence on the solution obtained by any nonlinear optimization program. Except for a few experiments, we have used the results of the greedy algorithm in

the previous section, with a somewhat judicious guess at the value of r , as the initial values for the nonlinear optimization.

3.2 Some Results

One of the values of interest is the optimized value of the parameter r . For function 1 the usual values tended to be around 0.1 to 0.2, although in some cases values outside that range were obtained; the smallest rms errors were obtained in that range. For function 2 much smaller values were obtained, generally in the range less than 0.05. For function 3, values in the range 0.20 to 0.30 were prevalent. For function 6 the value obtained in the one computation we carried out was more than 10. It is tempting to try to compare our results with the best values found for interpolation by [CF91], and with their formula for approximating the best value. For the moment we can say that for the most part the data do not seem contradictory, although for function 3 our values are somewhat smaller. For function 6, the value we obtained was in line with computational experience in [CF91] in that the value is quite large.

One very interesting aspect of the results of computing local minima of (5) is that, with the exception (and then not always) of computations involving fewer than 10 knots, the results involved near repeated knots, sometimes several different pairs with 20 or more knots, and sometimes triples of closely spaced knots. Because of the nonzero convergence tolerance for the optimization routine, by "near repeated" knots, we mean those that are within a distance consistent with the convergence tolerance. In some cases there were also other knots within distances of 0.02 or 0.03 for data in the unit square.

The occurrence of near multiple knots suggests that the method is trying to adapt to some behavior of the surface that cannot be approximated locally by a single multiquadric basis function. The behavior of a linear combination of multiquadric functions at points far away is essentially the same as a single multiquadric. Because of the local extremum of the multiquadric function near the knot point, it was not immediately clear what

could be achieved by a linear combination of multiquadrics at nearby knot points. Because of this, an investigation of the behavior of the surface defined by terms in the approximation (1) corresponding to the near repeated knots was undertaken, and in particular, comparison with the surface defined by a single multiquadric having the knot point at the average of the repeated knots, with coefficient equal to the sum of the coefficients for the repeated knots. Far away, the behavior of the composite function must be, and is seen to be, essentially similar to a single multiquadric. In the vicinity of the knots (and not necessarily just between them) the behavior can be very different.

Near multiple knots result in the coefficient matrix being poorly conditioned, which also allows for the possibility of large coefficients in the least squares solution of (3). We are unable to deduce for certain whether the closeness of knots is required in order for the coefficients to become large, or whether the closeness is required to obtain the required behavior in other ways. In one case we looked at, the knots are within 0.0035 of each other, the magnitude of the coefficients is on the order of 1125, and the condition number of the matrix is larger than 10^7 , some four orders of magnitude larger than needed for the magnitude of the coefficients since the data is on the order of one.

It seems to be true that the most deviant behavior of the sum of the near multiple terms occurs when the sum of the coefficients for the nearby knots is relatively close to zero. As an example showing quite different behavior of the sum of the terms for two nearby knots from that of the average term, see Figure 2. Parts a and b show perspective plots of the two surfaces, while parts c and d show contours of the same two surfaces. The deviation is striking and make it seem reasonable that in order to capture local behavior, multiple knots are necessary since local behavior cannot be affected by basis functions that are associate with far away knots, and each basis function itself is locally a hyperboloid (of one sheet - no

saddles) in shape.

Finally, we give the results of optimizing on the knot locations and the value of r for the 50 knot approximation corresponding to Figure 1. The results are shown Figure 3, and reveal that while many knots have moved from their initial positions, their density still reflects the same general pattern. Noteworthy is the fact that there is only one cluster of near repeated knots, those being the three at about $(.44, .78)$, near the dip in the surface. Those three are clustered within a distance of less than 0.01, while there is another knot within a distance of less than 0.025. Finally we note that the rms error for the surface was improved from 0.0037 to 0.00023 by the optimization process; r changed from the initial 0.2 to 0.2389.

4.0 Variable Knot Locations Each with Variable Parameter

The computational experience gained in the variable knot case, and especially the near repeated knot phenomenon lead us to consider whether or not the near multiple knots were occurring because a single value of the parameter at all knot locations was not necessarily appropriate. Thus, we modified the algorithm to allow for an independent r value, r_k , to be associated with each knot. The implications for the rank of the system is again not known. It is, however, easy to find examples of different parameter values that lead to singular systems in the interpolation problem. We believe the least squares problem is more robust, and have found no troublesome cases during our investigation.

4.1 Some Results

We soon discovered that the use of variable parameter values did not alleviate the problem of near multiple knots in the optimized approximation. It is interesting that when multiple knots occur, the parameter values for those knots are invariably very close to having the same value. In fact, our limited experience seems to indicate that most knots tend to have similar values of the parameter, although there are generally a few that

take on smaller values than elsewhere.

Once again, the behavior of the surface in the vicinity of near multiple knots often reflects behavior that cannot be taken on by a single multiquadric. As an example of a different kind of behavior than illustrated by Figure 2, note that Figure 4 shows another case where the near double knot results in a surface that resembles a quadric with a dimple in it. The r_k values for the two knots are essentially the same.

For comparison purposes between the greedy algorithm, the variable knot and parameter algorithm, and the variable knot each with variable parameter value, we look at a case with a few knots. In Figure 5 we give the results of the greedy algorithm for the data set 3-1 with 12 knots and an initial knot separation of 0.2. Parts a-d are, respectively, the point and knot set, the parent surface, the approximating surface, and contours of the approximating surface. In Figure 6 the results of the variable knot and parameter algorithm are given; the initial values were those resulting in Figure 5. Parts a-d are, respectively, the point set, the parent surface, the approximating surface, and the initial and final knots locations. The improvement is clear. In Figure 7 we see the results of the variable knot, each with variable parameter value. The parts of the figure are the same as for Figure 6. Here the improvement is even more spectacular. The values of the multiquadric parameter and the rms errors at the data points and on the grid are given in Table 3.

Algorithm	r value(s)	rmse(data)	rmse(grid)
Greedy	0.3	0.0320	0.0341
Var kts, var r	0.158	0.0101	0.0119
Var kts, var r_k	0.12-0.66	0.0012	0.0023

Table 3: Data set 3-1 with 12 knots, initial separation of 0.2

The improvement in the rms errors with variable knots is

significant for this particular data set. In situations where the number of knots is sufficient to give a reasonable approximation we find the typical improvement in rms errors is about by a factor of 3-10 when variable knots and parameter values is allowed, and another factor of 3-10 when the parameter values are allowed to vary. This is, however, highly dependent on the parent surface, for example, the cliff surface approximations are improved by smaller factors, while the saddle surface approximations tend to be at the upper end of the scale.

It is interesting to compare the results on this particular example with those of [CF91] with interpolation to the same data. There it was found that the "best" value of the parameter r (that being about 0.33) lead an approximation (which is the sum of 100 multiquadric terms) which has an rms error of 0.0026. It is startling to see that the 12 term approximation derived using variable knots each with variable r has smaller rms error. We have not followed this line of investigation very far, but function 2 (cliff) is also approximated well using relatively few knots.

It appears that the use of variable knots can give a greatly improved approximation when using multiquadric functions with a fixed number of knots. When variable parameter values are allowed the complexity of evaluating the approximation is essentially unchanged and seems to be a worthwhile improvement also. While there is a possibility of variable parameter values resulting in ill conditioning of the system, this does not appear to be a real problem.

5.0 Conclusions and Suggestions for Further Research

The methods we have developed here appear to be very useful for the purposes we consider, that of approximating surfaces from scattered data efficiently for use in subsequent computations. Which of the three algorithms one might employ to obtain the approximation depends on several matters that are peculiar to the data being approximated, as well as the computational requirements and resources available. If a reasonable

approximation is required with no heavy burden on subsequent use, the greedy knot selection process will probably yield a suitable result. If the final use imposes a high value on efficiency of evaluation, no doubt use of the two schemes giving optimized knot locations will look attractive. From our modest experiments it seems that use of variable parameter values at the knots adds approximation power beyond its cost.

To begin with, it is desirable to carry out the investigation with many more sets of data. Exploration of the process as we have done here is very important, using known underlying surfaces being approximated for comparison purposes. However, ultimately the use of the scheme must be for approximation of data obtained experimentally, or from environmental measurements. This data is almost invariably subject to error. While we have done some experimentation with such data (e, the glacier data), much remains to be done.

There are a number of directions in which this research can be extended. One idea we have explored slightly is that of using some measure of smoothness of the surface, in connection with the rms error at the data points, to determine when to stop the knot addition process in the greedy scheme. A reasonable stopping criterion is a necessity in approximating real-world data, especially if the error characteristics are largely unknown. We have computed the approximate value of the thin plate functional for these surfaces with the idea that an significant increase in the value of the functional accompanied by only slight decrease in the rms error may signal that complexity is being added to the surface without actually improving the fit to the underlying surface by much. We believe it will probably be necessary to monitor the values over some small numbers of knots, say over 5 or so consecutive numbers of knots. We intend to explore this as a potential stopping criterion.

In certain sets of data it may be desirable to include a smoothing term along with the rms error at the data points as part of the objective function in the knot location optimization schemes. One could take the objective function to be a convex

combination of the rms error and the value of some functional related to smoothness of the surface, such as the thin plate functional. There could be several reasons for this being desirable, but one is that if there are relative voids in the data, addition of a smoothing term would tend to give some control over the behavior of the function in such regions. There are many unknown factors in such a process. There are numerous cases where such objective functions have been found useful. See, for example, [HS91].

The particular form of the measure of smoothness probably depends on the application, and the use of the thin plate functional, while convenient and useful in many cases, may not be the proper one for environmental applications, for example. For meteorological problems it has been found that functionals corresponding to higher powers of the Laplacian seem to be appropriate [FR90]. Whatever the form of the measure of smoothness, the appropriate choice of weighting between the rms errors and the smoothness will also have to be discovered.

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Figure Captions

All figures are oriented (sideways) as

a	b
c	d

Figure 1: a) The 500 data points and the subset of 50 of them chosen as knot points as generated by the greedy algorithm are shown. Minimum knot separation enforced was 0.05. Contours of the parent function sampled for the data are also shown. b) A perspective plot of the parent function, viewed from a point in the first quadrant. c) A perspective plot of the plot of the approximating multiquadric function computed as the least squares approximation. d) Contours of the approximating function.

Figure 2: The surface representing two terms corresponding to two nearly repeated knots in a least squares approximation with optimized knot locations. The region is above the $[0,1]^2$ square on which the surface is sampled. b) The surface derived by averaging the location of the two knots and adding the coefficients. c) Contours of the surface corresponding to the two terms in part a. d) The contours of the single multiquadric term in part b.

Figure 3: a) The parent surface sampled at the 500 points show in Figure 1a. b) The approximating least squares multiquadric with knots at the initial guess points, as in Figure 1a. c) The surface corresponding to the least squares approximation using the optimized knot locations. d) The initial guesses and the optimized knot locations.

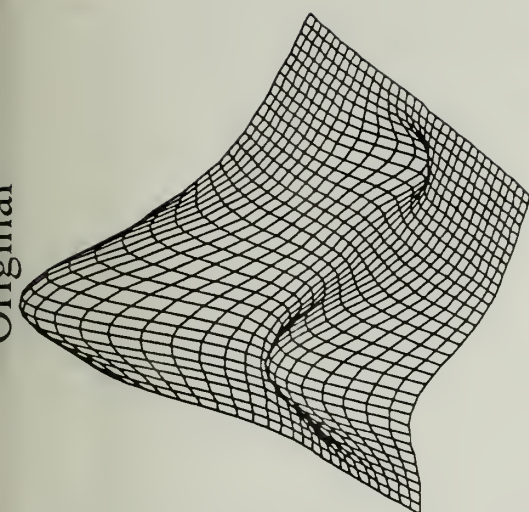
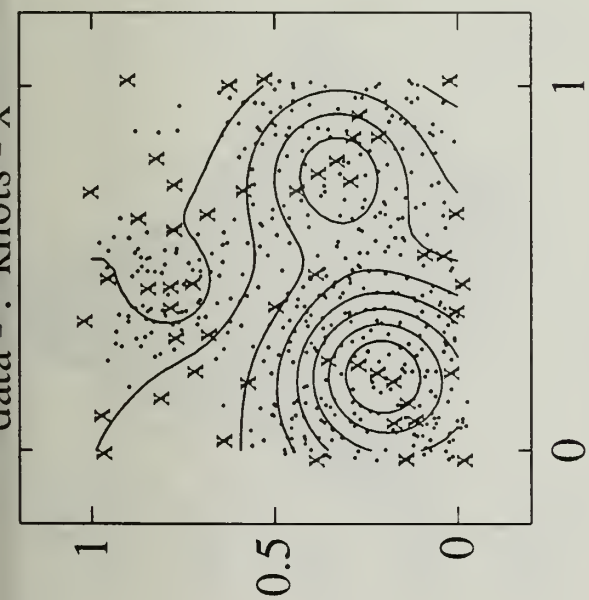
Figure 4: The surface representing two terms corresponding to two nearly repeated knots in a least squares approximation with optimized knot locations, each with optimized multiquadric parameter value; the optimized parameter values are essentially the same. The region is above the $[0,1]^2$ square on which the surface is sampled. b) The surface derived by averaging the location of the two knots and adding the coefficients. c) Contours of the surface corresponding to the two terms in part a. d) The contours of the single multiquadric term in part b.

Figure 5: a) The 100 data points and the subset of 12 of them chosen as knot points as generated by the greedy algorithm are shown. Minimum knot separation enforced was 0.2. Contours of the parent function sampled for the data are also shown. b) A perspective plot of the parent function, viewed from a point in the first quadrant. c) A perspective plot of the plot of the approximating multiquadric function computed as the least squares approximation. d) Contours of the approximating function.

Figure 6 a) The parent function which was sampled at the 100 points shown in Figure 5a. b) The least squares approximation constructed from the initial guess knot points, shown in part d as o's. c) The multiquadric approximation constructed from the optimized knot locations and (single) parameter value. d) The initial guess (o's) and optimized (x's) knot locations.

Figure 7: a) The parent function which was sampled at the 100 points shown in Figure 5a. b) The least squares approximation constructed from the initial guess knot points, shown in part d as o's. c) The multiquadric approximation constructed from the optimized knot locations and associated parameter values. d) The initial guess (o's) and optimized (x's) knot locations.

Original



Approximation

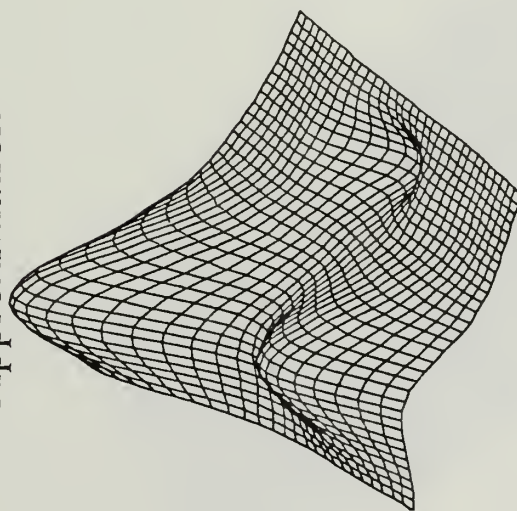
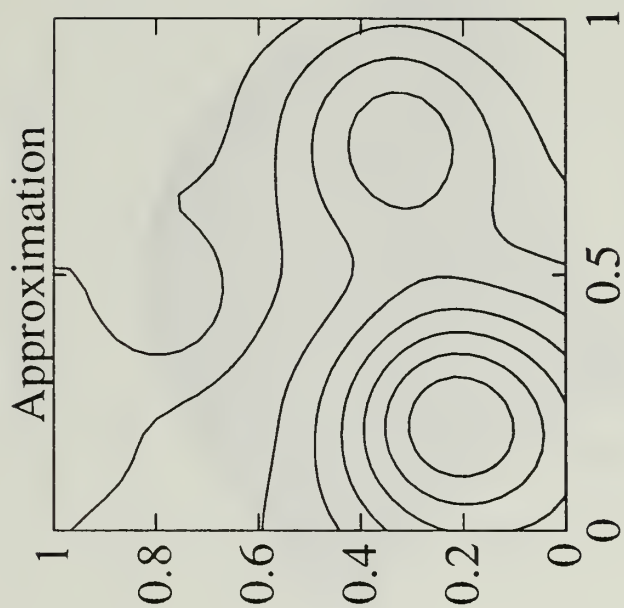
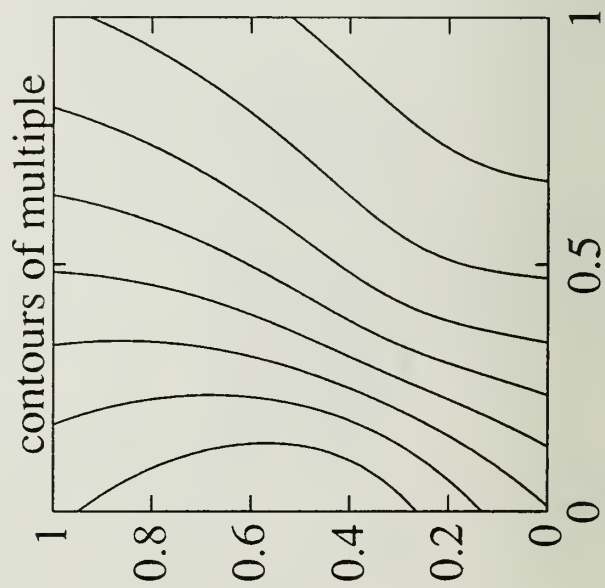
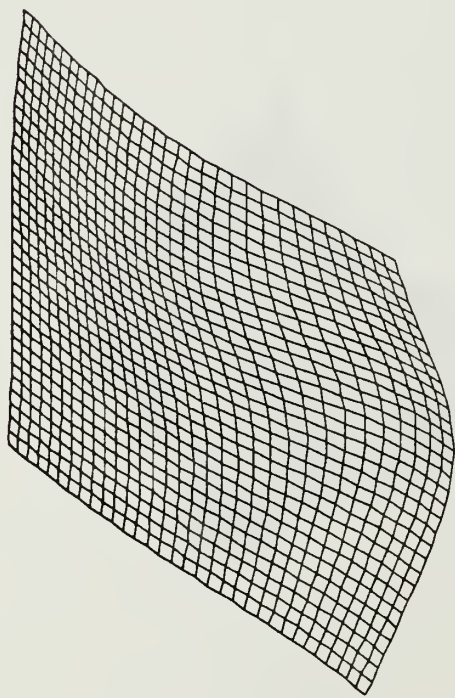
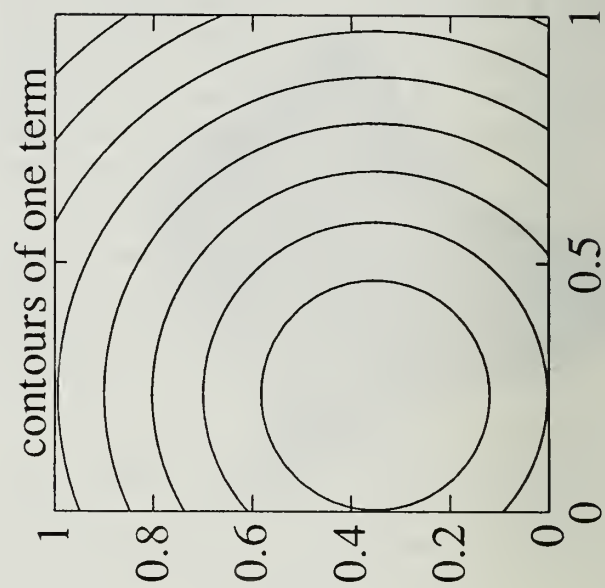
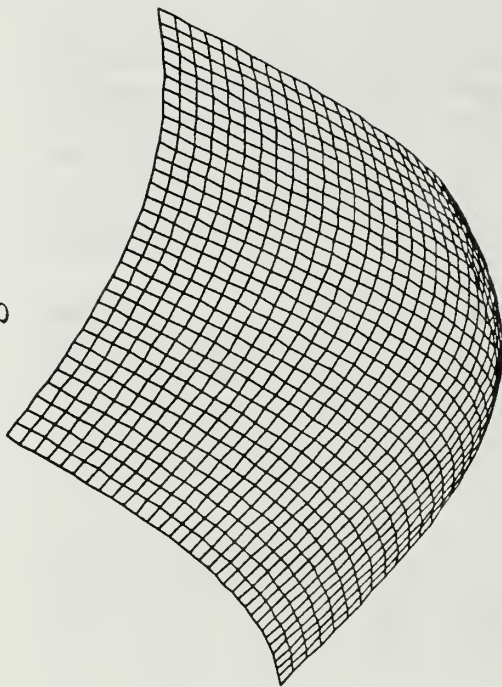


Figure 1

2 terms of multiple

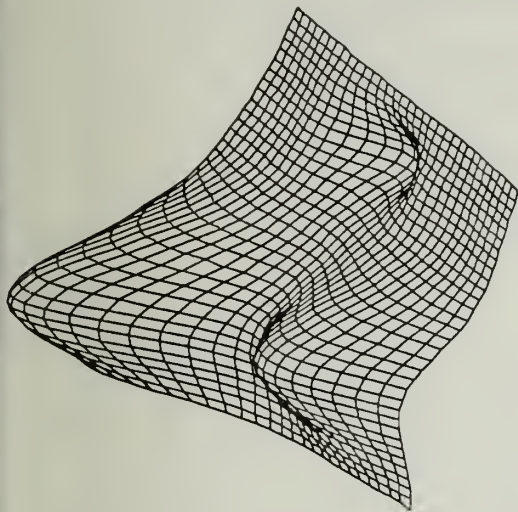
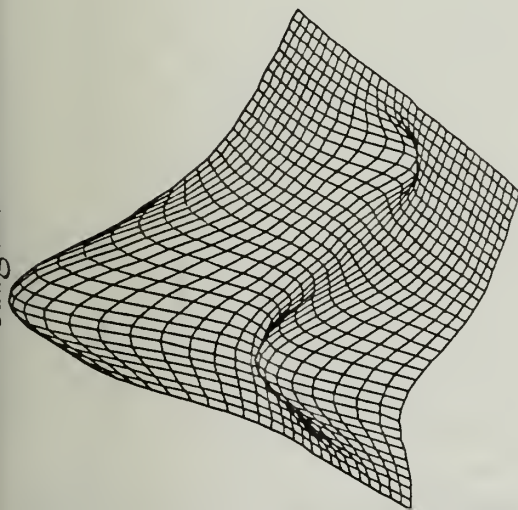


one average term



original

initial-50



optimized-50

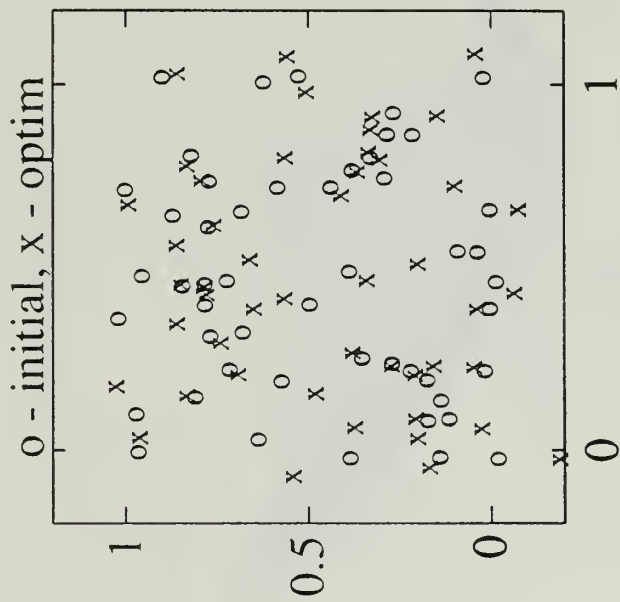
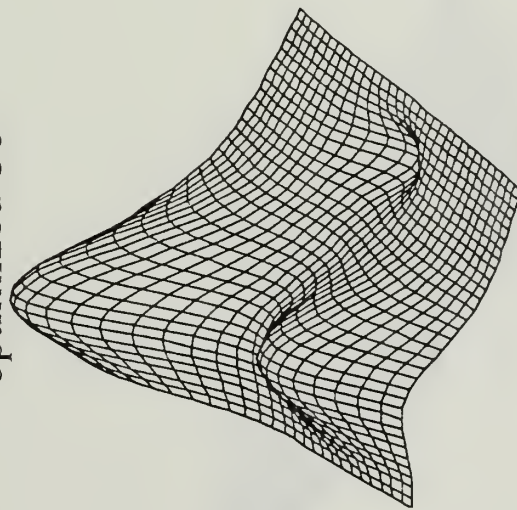
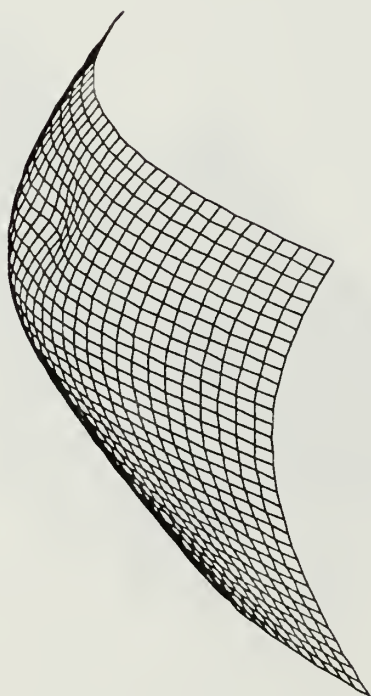
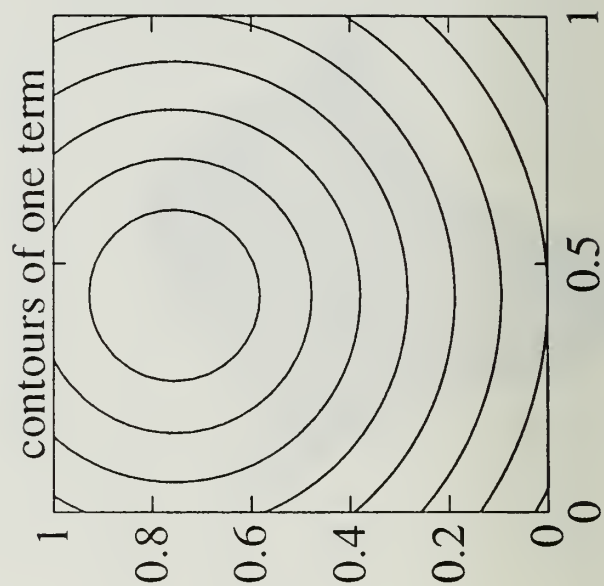
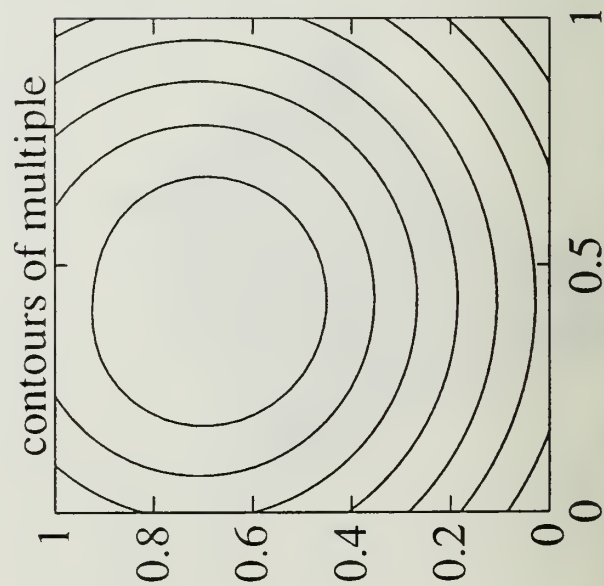
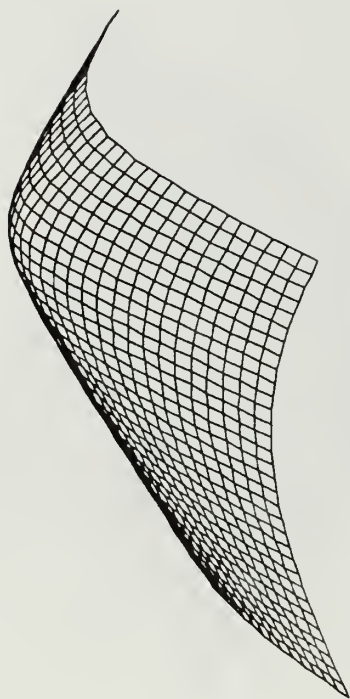


Figure 3

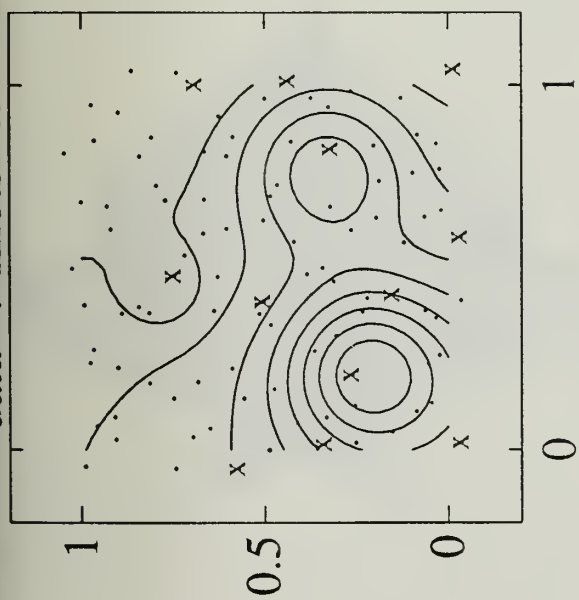
2 terms of multiple



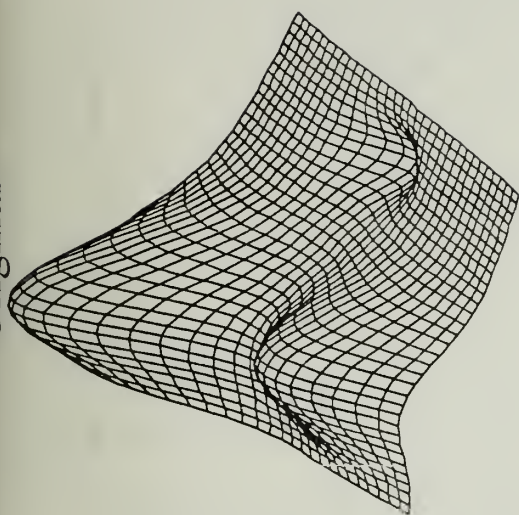
one average term



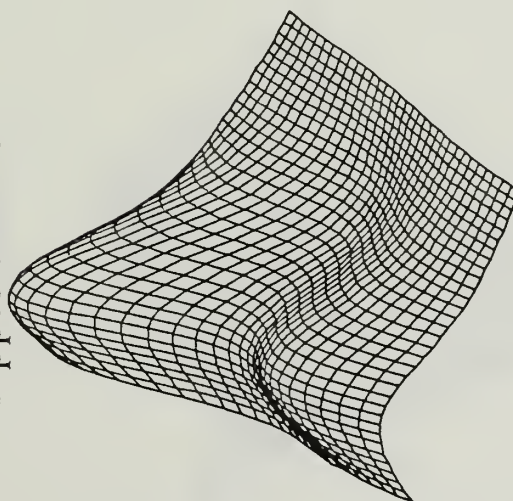
data - . knots - x



Original



Approximation



Approximation

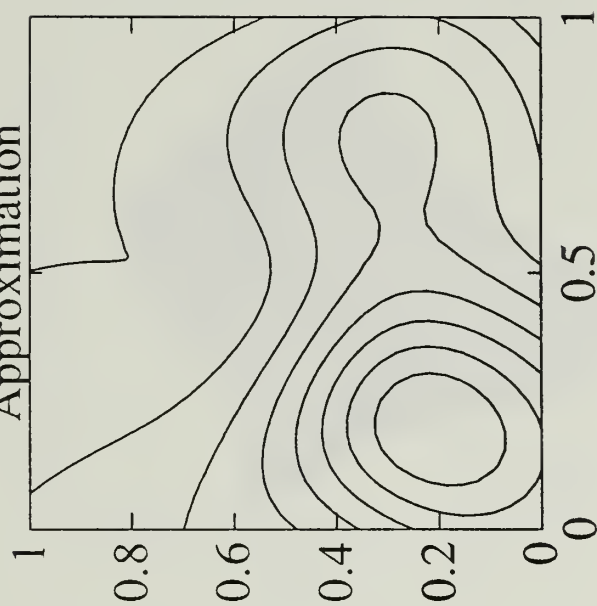
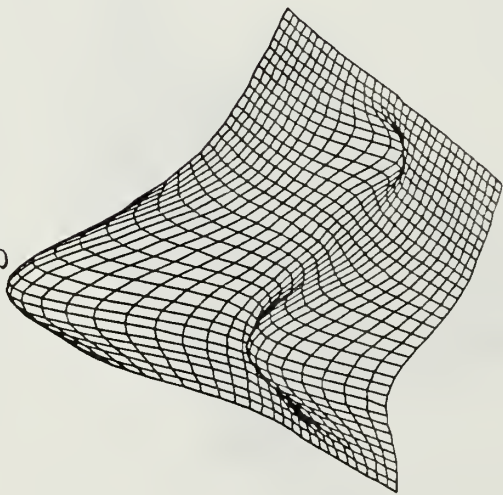
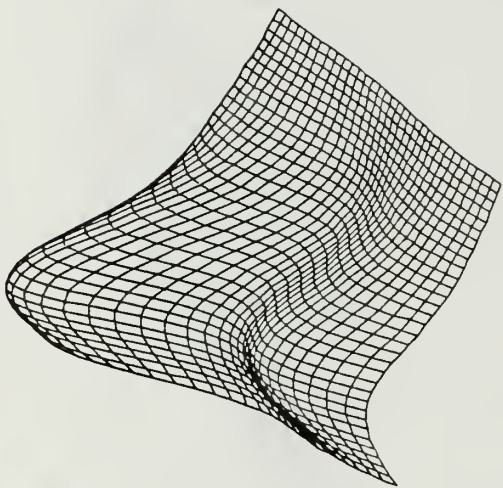


Figure 5

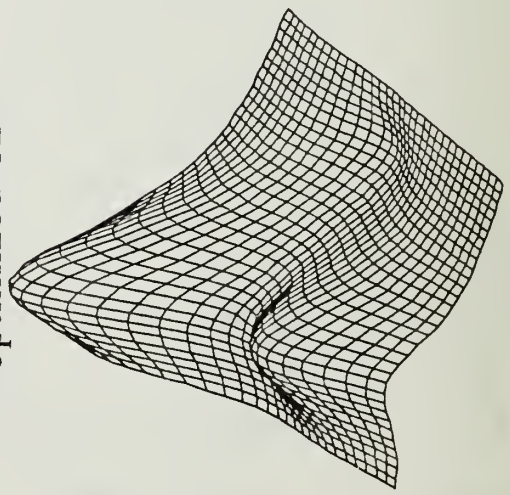
original



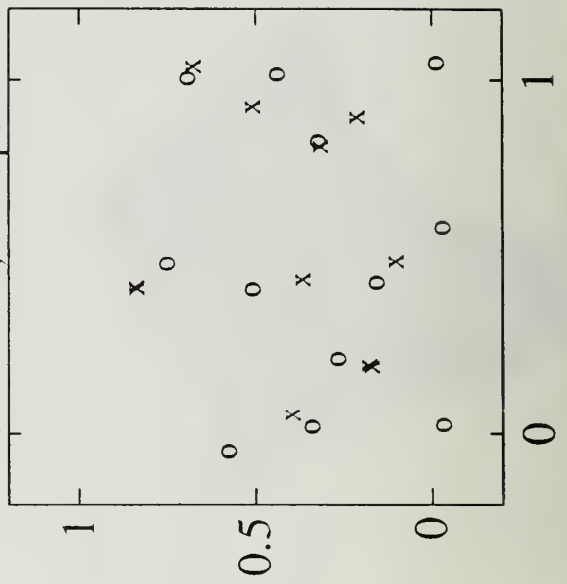
initial-12



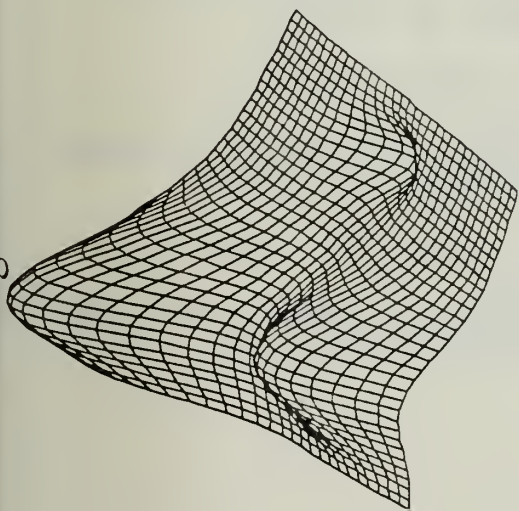
optimized-12



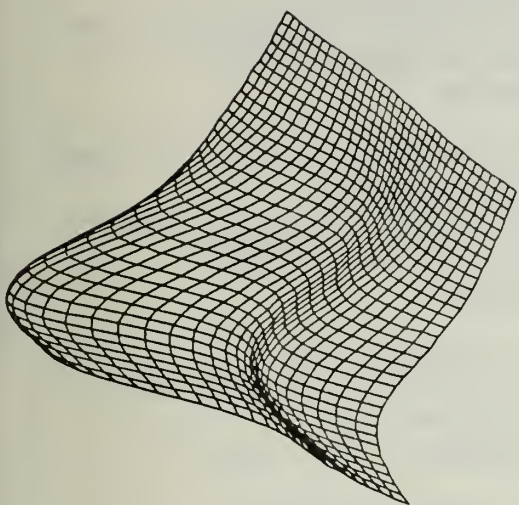
0 - initial, x - optim



original



initial-12



optimized-12

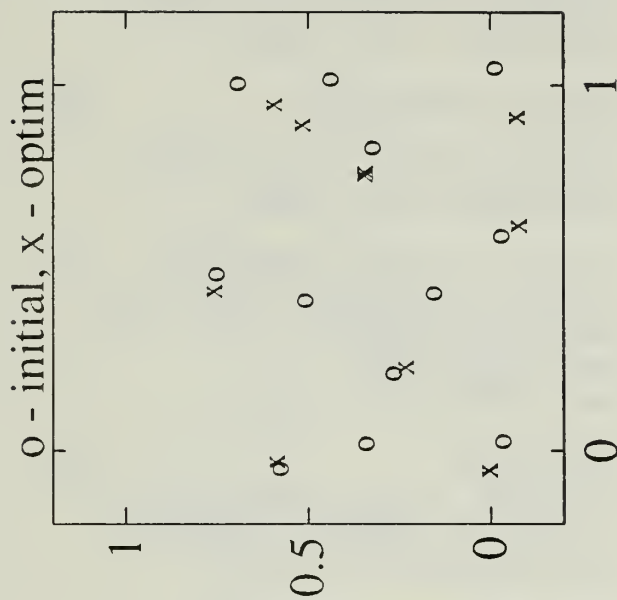
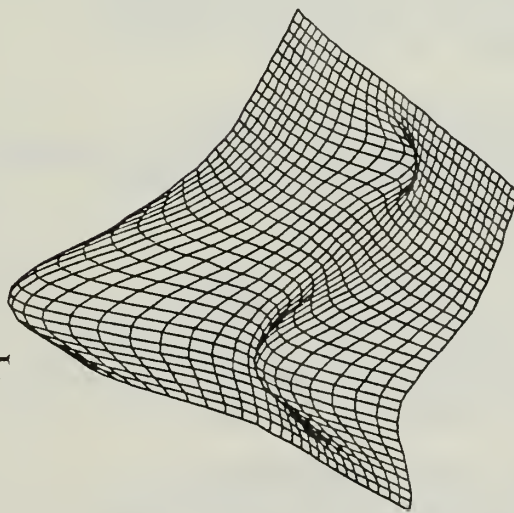


Figure 7

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